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Effective behavior of polycrystals that undergo martensitic phase transformation

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ABSTRACT

The shape-memory effect is the ability of a material to recover, on heating, apparently plastic deformations that it suffers below a critical temperature. These apparently plastic strains are not caused by slip or dislocation, but by deformation twinning and the formation of other coherent microstructures by the symmetry-related variants of martensite. In single crystals, these strains depend on the transformation strain and can be quite large. However, in polycrystals made up of a large number of randomly oriented grains, the various grains may not deform cooperatively. Consequently, these recoverable strains depend on the texture and may be severely reduced or even eliminated. Thus, the shape-memory behavior of polycrystals may be significantly different from that of a single crystal. We address this issue by studying some model problems in the setting of anti-plane shear.

1. INTRODUCTION

The shape-memory effect is the ability of a material to recover on heating, apparently plastic deformations that it suffers at low temperatures. At the heart of this phenomenon is a reversible martensitic phase transformation where the crystal lattice of the high temperature phase (*austenite*) has greater symmetry than that of the low temperature phase (*martensite*). As a result of the change in crystalline symmetry, there are several variants of martensite. Variants are identical lattices of martensite that are oriented differently with respect to the austenite. Thus, below the transformation temperature, a shape-memory material consists of a mixture of different martensitic variants, typically arranged in a fine-scale microstructure. When loads are applied, the material reduces its energy by converting from one variant to another, rearranging itself into a new microstructure and consequently suffering large apparently plastic deformations. On heating, each variant transforms back to the unique austenite, thereby recovering all deformation. Thus, the deformations that are recoverable by the shape-memory effect are exactly the deformations that a material can undergo by rearranging its martensitic variants.

For example, a single crystal consisting of only one grain subjected to shear can deform apparently plastically by deformation twinning. On heating, both twin variants transform to the austenite and all the shear strain is recovered. The maximum magnitude of the shear is determined by the transformation strains associated with the variants. The direction of shear is determined by the twinning plane and direction of twinning shear. In a polycrystal consisting of a large number of randomly oriented grains, the shear directions of the various grains do not coincide. Therefore, the recoverable shear that a polycrystal can undergo will at best be some average of the shears suffered by single crystals of different orientations. In fact, it could be worse. Since each grain is constrained by the surrounding grains, it can not deform freely. This suggests that the deformation of the polycrystal may be limited by the deformation of the worst-oriented grain. On the other hand, there is a possibility of finding a "percolating path of suitably oriented grains". This will increase the deformation of the polycrystal. The goal of this paper is to explore these competing effects. In particular, we wish to

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estimate the amount of recoverable strain in a polycrystal, and its dependence on polycrystalline texture, the change of crystalline symmetry and the transformation strain. Unfortunately, the problem is extremely difficult to address in any generality. In order to explore the interesting issues and the guiding principles, we decided to study some model problems in the setting of anti-plane shear. In this paper, we state the preliminary results of our investigations.

Experimentally, there are some alloys which display good shape-memory effect as single crystals, but only partial memory as polycrystals. Many alloys suffer inter-granular fracture at relatively low strains or after just a few shape-memory cycles. On the other hand, there are materials like Ni-50at%Ti which show excellent shape-memory effect even as polycrystals. They can undergo a large number of cycles and their recoverable strains are close to their transformation strains. We should mention here that our knowledge of experimental results is sketchy at best[1-9]. *One of our motivations for presenting our partial results to a wide audience is the hope that knowledgeable readers will educate us about experiments.*

In the last few years, there has been considerable theoretical work on materials that undergo martensitic transformations[10-19]. An important idea is a stored energy density function that depends on the deformation gradient and the temperature. Below the critical temperature, the energy density has multiple wells corresponding to the different martensitic variants. Minimizing this energy leads to fine-scale microstructure. The macroscopic behavior of the crystal is described by a relaxed or effective energy which takes into account the fine-scale microstructure. The recoverable deformations or strains of the shape-memory effect correspond to flat or degenerate regions of this effective energy. Up to now, the investigation of this model has been limited to single crystals. On the other hand, a lot is known about polycrystals made from materials that do not undergo martensitic transformation[20-24]. The goal of this work is to link these two areas of investigation.

2. MODEL PROBLEMS IN ANTI-PLANE SHEAR

2.1. Preliminaries

We consider a planar domain Ω in two-dimensions and limit our attention to "out-of-plane" deformations. The position vector is $x = \{x_1, x_2\}$and the deformation $\eta(x)$ is a real-valued function. We describe the orientation of the grains in a polycrystal by a spatially dependent rotation $R(x)$ which gives the orientation of the grain situated at position x. For a typical polycrystal, $R(x)$ is piecewise constant. For a single crystal, the orientation function $R(x)$ is equal to the identity matrix, $\mathbb{1}$, everywhere.

We fix the temperature at a value well below the transformation temperature and assume that there is a stored energy function ϕ that depends only on the deformation gradient, which is the vector $\nabla\eta = \left\{ \frac{d\eta}{dx_1}, \frac{d\eta}{dx_2} \right\}$. The total energy of a polycrystal with orientation function $R(x)$ subjected to a deformation η is given by $\int_\Omega \phi\big(R(x)\nabla\eta\,(x)\big)\,dx$. Our starting point is the hypothesis that the crystal assumes the configuration that minimizes the total energy for a given boundary condition. It is well-known that this minimization problem gives rise to fine-scale microstructure.

For a given polycrystal, we define the **effective energy** as the function $\bar{\phi}(f)$ which gives the spatially averaged energy of the polycrystal when the average or macroscopic strain is f. Formally,

$$\bar{\phi}(f) \stackrel{\text{def}}{=} \inf_{\eta|_{\partial\Omega} = f \cdot x} \left\{ \frac{1}{\text{Vol}\,\Omega} \int_{\Omega} \phi\big(R(x)\,\nabla\eta(x)\big)\,dx \right\}.$$

$\bar{\phi}$ takes into account the effect of microstructure as well as polycrystalline texture. It describes the macroscopic or effective behavior of the polycrystal.

We say that a polycrystal is **isotropic** if $\bar{\phi}(f) = \bar{\phi}(Qf)$ for all rotations Q and for all vectors f.

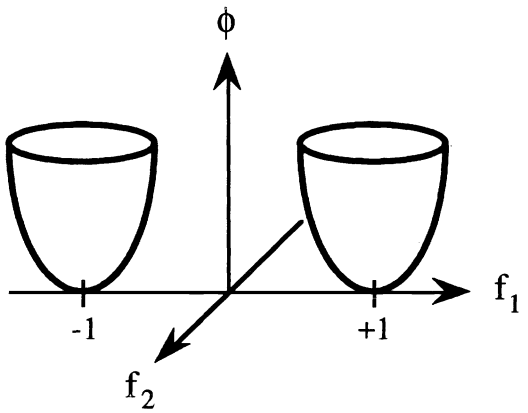

Figure 1. The stored energy density of the two variant material.

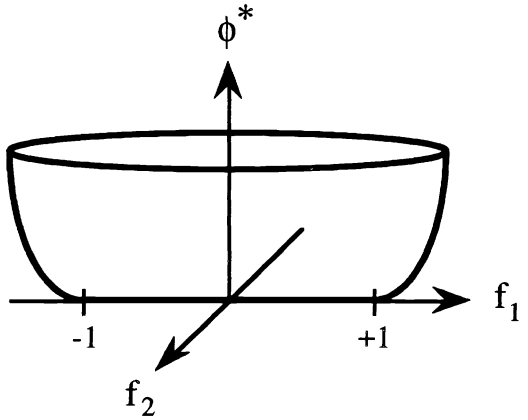

Figure 2. The effective energy of a single crystal of the two variant material.

2.2. The Two Variant Material

Consider a material with the stored energy density, $\phi(f) = \frac{1}{2} \min \{ (f_1 \pm 1)^2 + f_2^2 \}$. This function is shown in Figure 1. It consists of two minima at the points $f = \{\pm 1, 0\}$. It corresponds to the energy function of a (fictitious) material with two variants, having transformation or stress-free strain of $\{\pm 1, 0\}$.

In a single crystal (i.e., $R(x) = \mathbb{1}$ everywhere), the effective energy is exactly equal to the convexification of the energy ϕ. For the two variant material, it is shown in Figure 2 and is equal to one half the square of the distance from the line segment joining $\{-1,0\}$ and $\{1,0\}$. In particular, notice that $\phi^* = 0$ on the line joining $\{-1,0\}$ and $\{1,0\}$. This is very easy to understand. If we prescribe boundary conditions such that the average strain lies on that line (e.g. $\eta(x) = 0$ for $x \in \partial\Omega$), the material just makes a mixture of the two variants in suitable proportions and reduces its total energy to zero. Thus, we see that we can plastically deform a single crystal along this line and it will respond by simply rearranging its variants. This line corresponds to the set of all recoverable strains of the shape-memory effect.

Let us now consider a polycrystal of this material. We have been able to prove that the effective energy of any isotropic polycrystal of the two variant material is bounded below by a quartic function near the origin. Consequently, the effective energy of an isotropic polycrystal has no flat or degenerate region. This implies that an isotropic polycrystal of the two variant material **can not** undergo any deformation by simply rearranging its variants. In the context of shape-memory effect, this means that there is no recoverable apparently plastic deformation in isotropic polycrystals of this type. Thus, an isotropic polycrystal of the two variant material **loses** all the shape-memory behavior that characterizes the single crystal.

We have also been able to show that the effective energy is sub-quadratic at the origin. Therefore, the second derivatives of $\bar{\phi}$ which correspond to the linear elastic moduli are zero. Thus, though the energy has no flat region, the polycrystal is extremely soft at the origin. We believe that this kind of softening contributes to the fact that the stress-strain curves of a polycrystal are more rounded and smooth compared to those of a single crystal.

2.3. The Four Variant Material

Consider a material with the stored energy density, $\phi(f) = \frac{1}{2} \min \{ (f_1 \pm 1)^2 + (f_2 \pm 1)^2 \}$. This energy function consists of four minima at the points $f = \{\pm 1, \pm 1\}$. These are the bold points shown in Figure 3.

In the case of a single crystal, the effective energy is zero on the square shown in Figure 3 and grows quadratically out of it. The set of all deformations that a single crystal of the four variant material can undergo by simply rearranging its microstructure is described by the square with side-length two centered at the origin. In other words, this square describes the set of all deformations recoverable by the shape-memory effect.

A polycrystal of this material consists of many grains, each with a different orientation. Consider a grain with orientation R. It's effective energy is zero on the rotated square in the

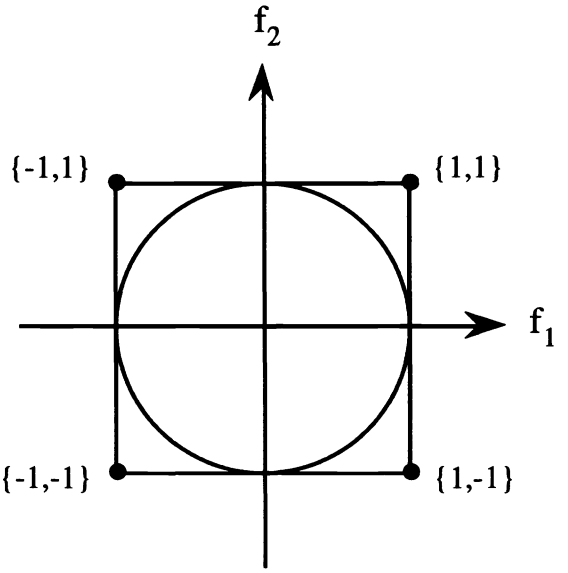

Figure 3. The deformation gradient space corresponding to the four variant material. The four bold dots at the corners of the square are the transformation or the stress-free strain of the four variants. The effective energy of a single crystal is zero on the square and grow quadratically out of it. The effective energy of any polycrystal of this four variant material will be zero on the inscribed circle.

f_1-f_2-plane: this rotated square is obtained by rotating the "single-crystal-square" (see Figure 3) by R about the origin. Now, if f lies in the inscribed circle in Figure 3, then f is contained within each "rotated square" and the effective energy of each grain is zero at f. Therefore, for any polycrystal of the four variant material, the effective energy is zero in this inscribed circle, i.e., in the circle $|f| \leq 1$. In other words, irrespective of the texture (and in particular in the isotropic case), polycrystals of this four variant material **can** undergo deformation by simply rearranging its variants and **will** display the shape-memory effect.

We suspect that for some polycrystals, i.e. for some orientation functions R(x), the set on which the effective energy $\overline{\phi}$ is zero is larger than the circle. It would be interesting to estimate the set on which $\overline{\phi} = 0$ in terms of R(x). That would correspond to studying the effect of texture on the recoverable strain.

3. DISCUSSION AND CONCLUSION

We have considered two model problems in anti-plane shear. For the two variant material, an isotropic polycrystal **loses** all shape-memory effect that is present in a single crystal. On the contrary, for the four variant material, every polycrystal **retains** a significant amount of the shape-memory effect. We are currently trying to extend these calculations to a fully 3 dimensional model. For now, the lesson we draw is the following: the number of distinct martensitic variants is as crucial as the transformation strain in determining polycrystalline shape-memory behavior. In particular, it is important to have a large number of variants for good shape-memory behavior in polycrystals. This entails a large change in

symmetry during the martensitic transformation. Thus, we would like to have high symmetry in the austenite and low symmetry in the martensite. This idea is strengthened by some results of Bhattacharya[13]. Using certain calculations about self-accommodation, he argues that the austenite of any shape-memory materials must have cubic symmetry, which is maximal. Our model problems suggest that, in addition, the symmetry of the martensite should preferably be orthorhombic or monoclinic for good shape-memory behavior in the polycrystalline state.

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